

Effect of Compressibility on the Annihilation Process

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Abstract

Annihilation processes, where the reacting particles are influenced by some external advective field, are one of the simplest examples of nonlinear statistical systems. This type of processes can be observed in miscellaneous chemical, biological or physical systems. In low space dimensions usual description by means of kinetic rate equation is not sufficient and the effect of density fluctuations must be taken into account. Using perturbative renormalization group we study the influence of random velocity field on the kinetics of single-species annihilation reaction at and below its critical dimension $d_c = 2$. The advecting velocity field is modelled by the self-similar in space Gaussian variable finite correlated in time (Antonov-Kraichnan model). Effect of the compressibility of velocity field is taken into account and the model is analyzed near its critical dimension by means of three-parameter expansion in ϵ , Δ and η . Here ϵ is the deviation from the Kolmogorov scaling, Δ is the deviation from the (critical) space dimension 2 and η is the deviation from the parabolic dispersion law. Depending on the value of these exponents and the value of compressibility parameter α ,

the studied model can exhibit various asymptotic (long-time) regimes corresponding to the infrared (IR) fixed points of the renormalization group. The possible regimes are summarized and the decay rates for the mean particle number are calculated in the leading order of the perturbation theory.

1 Introduction

Variety of chemical reactions occur in fluid environment and represents very important subject in various chemical, biological or physical systems [1, 2, 3]. In these processes the reacting particles are affected not only by the diffusion motion but also by the external fluid flow. The usual approach to such reactive flows is based on some combination of reaction-transport equations.

In this work we will concentrate on the study of the annihilation reaction $A + A \rightarrow \emptyset$, which is the paradigmatic model for the reaction-diffusion processes. For this type of reaction in low space dimensions the usual description by means of kinetic rate equation is not sufficient and the effect of density fluctuations must be taken into the account [4]. It can be shown that the upper critical dimension for this process, even in the absence of advective flow, is two due to the density fluctuations. A renormalization group treatment was successfully applied for different choices of reactive flow, e.g. time-independent random drift [5], velocity field described by stochastic Navier-Stokes equation [6] or short-range correlated potential disorder [7]. Often large differences are observed in relation to the experiment and their origin can be caused by the presence of large-scale anisotropies, effect of compressibility or parity violation. There are important differences [8, 9] between advection of scalar quantities like density on one hand and like tracer (temperature, concentration) on the other by compressible versus incompressible flow. It was shown that compressibility could lead to the slowing of transport process for scalar admixture and also to the enhancement of intermittent phenomena. These effects might be understood as a result of inhibition of separation between particle trajectories and therefore we expect that reacting particles would spent effectively more time in the mutual vicinity than in the incompressible case. Hence in this case we expect the faster decay rate than for the incompressible case. Hence it would be desirable to support such naive picture in more quantitative manner. In order to do that we will apply Antonov-Kraichnan model [10, 11] for describing advection of

reactive A particles and we will present renormalization group (RG) study in the vicinity of its critical dimension $d_c = 2$. In the one-loop order all relevant physical quantities are calculated and contrary to the incompressible case it is found out, that already in the one-loop approximation fluctuations of the velocity field affect the renormalization of the rate constant.

After brief description of the model in Sec. 2, results of RG calculations are presented in Sec. 3. In Sec. 4 possible large-scale regimes are listed and their physical interpretation is concluded in Sec. 5.

2 Field-theoretic model

Field-theoretic action for the annihilation reaction process $A + A \xrightarrow{K_0} \emptyset$ can be obtained in the straightforward way [12] employing Doi approach [13]. It can be written in the following standard form

$$S_1 = - \int_0^\infty dt \int d\mathbf{x} \left\{ \psi^\dagger \partial_t \psi - D_0 \psi^\dagger \nabla^2 \psi + \lambda_0 D_0 [2\psi^\dagger + (\psi^\dagger)^2] \psi^2 \right\} + n_0 \int d\mathbf{x} \psi^\dagger(\mathbf{x}, 0), \quad (1)$$

where D_0 is the diffusion constant of reacting particles, and because of dimensional reasons we have rewritten product $\lambda_0 D_0$ instead of the rate constant K_0 . Last term in the action stands for the initial conditions, which are traditionally chosen in the form of Poisson distribution.

In compressible velocity field, there are two types of diffusion-advection problems: advection of a density field and advection of a tracer field [14]. Here, the case of advection of a density field will be analyzed [15]. In the action (1) this corresponds to the replacement $\psi^\dagger \partial_t \psi \rightarrow \psi^\dagger [\partial_t \psi + (\nabla \cdot \mathbf{v}) \psi]$, where $\mathbf{v} = \mathbf{v}(\mathbf{x}, t)$ is the advecting velocity field. According to [11] let us assume that \mathbf{v} is a random Gaussian variable with zero mean and the correlator (in the frequency-momentum representation)

$$\langle v_{0i} v_{0j} \rangle_0 = \frac{g_0 D_0^3 k^{2-2\Delta-2\epsilon-2\eta}}{\omega^2 + (u_0 D_0 k^{2-\eta})^2} [P_{ij}(\mathbf{k}) + \alpha Q_{ij}(\mathbf{k})], \quad (2)$$

where g_0 is the coupling constant, the exponents ϵ, Δ and η play the role of small expansion parameters. They could be regarded as an analog of the expansion parameter $\epsilon = 4 - d$ used in the theory of critical phenomena. However, in this paper ϵ should be understood as deviation of exponent of the power law from that of the Kolmogorov scaling [16], whereas Δ is defined

as the deviation from the space dimension two via relation $d = 2 + 2\Delta$, and the exponent η is related to the reciprocal of the correlation time at the wave number k . The parameter u_0 serves for labeling of the fixed points and it can be interpreted as a ratio of velocity correlation time and the scalar turnover time [17]. In (2) besides the standard (incompressible) transverse projection operator $P_{ij}(\mathbf{k}) = \delta_{ij} - k_i k_j / k^2$ the longitudinal projector $Q_{ij}(\mathbf{k}) = k_i k_j / k^2$ has been introduced. The positive (necessary for positive definiteness of the correlator $\langle vv \rangle$) parameter α represents the degree of compressibility. The incompressible case is obtained by the setting $\alpha = 0$.

The Antonov-Kraichnan model for the advection field \mathbf{v} contains two cases of special interest:

- (a) in the limit $u_0 \rightarrow \infty, g'_0 \equiv g_0/u_0^2 = \text{const}$ we get the 'the rapid-change model' $D_v(\omega, \mathbf{k}) \rightarrow g'_0 D_0 k^{-2-2\Delta-2\epsilon+\eta}$, which is characterized by the white-in-time nature of the velocity correlator.
- (b) limit $u_0 \rightarrow 0, g''_0 \equiv g_0/u_0 = \text{const}$ corresponds to the case of a frozen velocity field $D_v(\omega, \mathbf{k}) \rightarrow g''_0 D_0^2 \pi \delta(\omega) k^{2\Delta-2\epsilon}$, when the velocity field is quenched (time-independent).

The averaging procedure with respect to the velocity field $\mathbf{v}(x)$ may be performed with the aid of the following action functional

$$S_2 = -\frac{1}{2} \int dt d\mathbf{x} \int dt' d\mathbf{x}' \mathbf{v}(t, \mathbf{x}) D_v^{-1}(t - t', \mathbf{x} - \mathbf{x}') \mathbf{v}(t', \mathbf{x}'), \quad (3)$$

where D_v^{-1} is the inverse correlator (2) (in the sense of the Fourier transform). The expectation value of any relevant physical observable may be calculated using the complete weight functional $\mathcal{W}(\psi^\dagger, \psi, \mathbf{v}) = e^{S_1 + S_2}$, where S_1 and S_2 are the action functionals (1) and (3).

3 UV renormalization

The inclusion of longitudinal part Q into the correlator for velocity field does not affect the renormalization group analysis developed for the such model [18]. Therefore we just mention main steps of theoretical description and deviations from it caused by compressibility violation. All canonical dimensions of fields and parameters are listed in Tab. 1. The only difference with the incompressible case is that now the velocity field has to be renormalized [11]. Following [6, 11, 18] it is easy to prove that the model under

Q	ψ	ψ^\dagger	v	D_0	u_0	λ_0	g_0	α, g, u, λ
d_Q^k	d	0	-1	-2	η	-2Δ	$2\epsilon + \eta$	0
d_Q^ω	0	0	1	1	0	0	0	0
d_Q	d	0	1	0	η	-2Δ	$2\epsilon + \eta$	0

Table 1: Canonical dimensions for the parameters and fields of the model

consideration is multiplicatively renormalizable and can be made UV finite by the following renormalization prescription

$$D_0 = DZ_D, \quad g_0 = g\mu^{2\epsilon+\eta}Z_g, \quad u_0 = u\mu^\eta Z_u, \quad \lambda_0 = \lambda\mu^{-2\Delta}Z_D^{-1}Z_\lambda, \quad \mathbf{v}_0 = \mathbf{v}Z_v \quad (4)$$

with the additional constraints between them

$$Z_g Z_D^3 = 1, \quad Z_u Z_D = 1, \quad Z_g Z_D^3 = Z_v^2, \quad (5)$$

which are the consequences of the absence of renormalization of non-local term (2). Non-local character of the velocity correlator is caused by the nontrivial correlations in momentum and frequency scales. The total renormalized action can be written as

$$\begin{aligned} S_R(\psi^\dagger, \psi, \mathbf{v}) &= - \int_0^\infty dt \int d\mathbf{x} \left\{ \psi^\dagger \partial_t \psi - \psi^\dagger D Z_D \nabla^2 \psi + \psi^\dagger Z_v (\nabla \cdot \mathbf{v} \psi) \right\} - \\ &- Z_\lambda D \lambda [2\psi^\dagger + \psi^{\dagger 2}] \psi^2 \Big\} - \int dt d\mathbf{x} \int dt' d\mathbf{x}' \frac{v D_v^{-1} v}{2} + \\ &+ n_0 \int d\mathbf{x} \psi^\dagger(\mathbf{x}, 0). \end{aligned}$$

The perturbative calculation of the renormalization constants in dimensional regularization with the use minimal subtraction (MS) scheme is straightforward [19]. We restrict ourselves to the first order in perturbation theory and this approximation already contains first nontrivial effect of the compressibility. It can be seen from the perturbation expansion of the one-particle irreducible function $\Gamma_{\psi^\dagger \psi^2}$ (known as interaction vertex)

$$\Gamma_{\psi^\dagger \psi^2} |_{\omega=0, p^2=0} = -4D\lambda Z_\lambda \mu^{-2\Delta} + \frac{1}{2} \text{ (loop diagram) } + \frac{1}{2} \text{ (triangle diagram) }, \quad (6)$$

where higher order terms in coupling constants were neglected. The first graph on the r.h.s. of (6) physically represents process of density fluctuations that account for annihilating of two particles. It is easy to see that transverse character (equivalent statement to the incompressibility condition for velocity field \mathbf{v}) of propagator $\langle vv \rangle$ leads to UV divergent contribution of the second graph in (6), whereas for the models with incompressible velocity field \mathbf{v} it leads to UV convergent contribution. Physically this graph can be interpreted as an attracting process that brings together particles into a sink of compression, which can lead to effective increase of the reaction rate as will be pointed later. In the MS scheme the renormalization constants in one-loop calculation obtain the following form

$$Z_D = 1 - \frac{g}{16\pi u(1+u)\epsilon} \left[1 + \alpha - \frac{2\alpha}{1+u} \right], \quad (7)$$

$$Z_v = 1 + \frac{\alpha g}{16\pi u(1+u)^2\epsilon}, \quad (8)$$

$$Z_\lambda = 1 - \frac{\lambda}{4\pi\Delta} - \frac{\alpha g}{16\pi u(1+u)\epsilon}, \quad (9)$$

and from relations (5) constants Z_u and Z_g can be calculated. Limiting case $\alpha = 0$ agrees with the results (to the one-loop precision) for incompressible case [18] and case $g = 0$ leads to the presence of only density fluctuations [4].

From the relations (4) and (5) the beta functions β_g, β_u and β_λ are obtained via the standard definition $\beta_g = \mu \partial_\mu g|_0$ (the subscript "0" refers to partial derivatives taken at fixed values of the bare (unrenormalized) parameters)

$$\beta_g = g[-2\epsilon - \eta + 3\gamma_D - 2\gamma_v], \quad \beta_u = u[-\eta + \gamma_D], \quad \beta_\lambda = \lambda[2\Delta - \gamma_\lambda + \gamma_D], \quad (10)$$

where the anomalous dimensions γ_F are defined as [19]

$$\gamma_F = \mu \partial_\mu \ln Z_F|_0 = (\beta_g \partial_g + \beta_u \partial_u + \beta_\lambda \partial_\lambda) \ln Z_F. \quad (11)$$

It was conjectured [11, 17, 20], that up to the two-loop calculations there is no direct influence of the parameter η on the anomalous dimensions. Hence one can use in the actual calculations of the Feynman graphs different values of η . In our calculations the simplest choice $\eta = 0$ was applied. Finally substituting

(9) into the definition (11) the anomalous dimensions are obtained

$$\gamma_D = \frac{g}{8\pi u(1+u)} \left[1 + \alpha - \frac{2\alpha}{u+1} \right], \quad \gamma_v = -\frac{\alpha g}{8\pi u(1+u)^2},$$

$$\gamma_\lambda = \frac{\alpha g}{8\pi u(1+u)} - \frac{\lambda}{2\pi}.$$

4 IR stable regimes

We are interested in the IR asymptotics of small momentum \mathbf{p} and frequencies ω of the renormalized functions or, equivalently, large relative distances and time differences in the (t, \mathbf{x}) representation. Such a behavior is governed by the IR-stable fixed point $g^* = (g_1^*, u^*, \lambda^*)$, which are determined as zeroes of the β functions (10): $\beta(g^*) = 0$. It is said, that the fixed point g^* is IR stable, if real parts of all eigenvalues of the matrix $\Omega_{ij} \equiv \partial\beta_i/\partial g_j|_{g=g^*}; i, j \in \{g, u, \lambda\}$ are strictly positive.

The simplest way to find the average number density $n(t) = \langle \psi(t) \rangle$ is to calculate it from the stationarity condition of the functional Legendre transform [21] of the generating functional obtained by replacing the unrenormalized action by the renormalized one in the weight functional [6]. This is a convenient way to avoid any summing procedures used [4] to take into account the higher-order terms in n_0 . For a spatially homogenous solution this leads to the rate equation with the initial condition $n(0) = n_0$ for the average number density $n(t) = \langle \psi(t) \rangle$

$$n(t) = \frac{n_0}{1 + 2\lambda u D t \mu^{-2\Delta} n_0},$$

where n_0 is the initial number density. Since the fields ψ and ψ^\dagger are not renormalized, the Callan-Symanzik equation for the mean particle number is easily obtained by the standard procedure [6, 22]

$$\left[(2 - \gamma_D) t \frac{\partial}{\partial t} + \sum_g \beta_g \frac{\partial}{\partial g} - d n_0 \frac{\partial}{\partial n_0} + d \right] n(t, \mu, D, n_0, g) = 0$$

Solving it by the means of characteristics it can be shown (details will be published elsewhere [23]) that the value of the decay exponent β defined through the asymptotic relation : $n(t) \underset{t \rightarrow \infty}{\sim} t^{-\beta}$ is given by the expression

$$\beta = 1 + \frac{\gamma_\lambda^*}{2 - \gamma_D^*}.$$

Note that in contrast to the previous studies [6, 18] here we have to deal only with the three-charges' $\{g, u, \lambda\}$ theory. Passive character (no backward influence on the advecting field) of the reacting particle manifests itself also in the relations $\partial_\lambda \beta_g = \partial_\lambda \beta_u = 0$ resulting from (9) and (10). These relations greatly simplify calculation of the eigenvalues of ω_{ij} matrix.

Detailed analysis of fixed point structure reveals that studied system can exhibit one of ten possible IR regimes listed below. First let us consider the "rapid-change model" ($u \rightarrow \infty$). Introducing convenient variables $w = 1/u$, $g' = g/u^2$, the corresponding β functions can be written in the form

$$\beta_{g'} = g'[-2\epsilon + \eta + \gamma_D - 2\gamma_v], \quad \beta_w = w[\eta - \gamma_D], \quad \beta_\lambda = \lambda[2\Delta - \gamma_\lambda + \gamma_D],$$

where anomalous dimensions are

$$\gamma_D = \frac{g'}{8\pi(1+w)} \left[1 + \alpha - \frac{2\alpha w}{1+w} \right], \quad \gamma_v = -\frac{\alpha g'}{8\pi(1+w)^2}, \quad \gamma_\lambda = \frac{\alpha g'}{8\pi(1+w)} - \frac{\lambda}{2\pi}.$$

The "rapid-change model" corresponds to the fixed point with the value $w^* = 0$. In this case four stable IR fixed points can be realized:

$$\begin{aligned} \textbf{FP 1:} \quad & g'^* = 0, \quad \lambda^* = 0; \\ & \Omega_1 = \eta - 2\epsilon, \quad \Omega_2 = \eta, \quad \Omega_3 = 2\Delta; \\ & \beta = 1; \\ \textbf{FP 2:} \quad & g'^* = 0, \quad \lambda^* = -4\pi\Delta; \\ & \Omega_1 = \eta - 2\epsilon, \quad \Omega_2 = \eta, \quad \Omega_3 = -2\Delta; \\ & \beta = 1 + \Delta; \\ \textbf{FP 3:} \quad & g'^* = \frac{8\pi(2\epsilon - \eta)}{1 + \alpha}, \quad \lambda^* = 0; \\ & \Omega_1 = 2\epsilon - \eta, \quad \Omega_2 = 2\eta - 2\epsilon, \quad \Omega_3 = 2\Delta + \frac{2\epsilon - \eta}{1 + \alpha}; \\ & \beta = \frac{2\alpha + 2 - 2\epsilon + \eta}{(1 + \alpha)(2 - 2\epsilon + \eta)}; \\ \textbf{FP 4:} \quad & g'^* = \frac{8\pi(2\epsilon - \eta)}{1 + \alpha}, \quad \lambda^* = 2\pi \left(2\Delta + \frac{-2\epsilon + \eta}{1 + \alpha} \right); \\ & \Omega_1 = 2\epsilon - \eta, \quad \Omega_2 = 2\eta - 2\epsilon, \quad \Omega_3 = -2\Delta - \frac{2\epsilon - \eta}{1 + \alpha}; \\ & \beta = \frac{2 + 2\Delta}{2 - 2\epsilon + \eta}. \end{aligned}$$

For the analysis of the regime $u \rightarrow 0$ (quenched velocity field) we introduce the new variable $g'' \equiv g/u$. Hence the corresponding β functions have the form

$$\beta_{g''} = g''[-2\epsilon + 2\gamma_D - 2\gamma_v], \quad \beta_u = u[-\eta + \gamma_D], \quad \beta_\lambda = \lambda[2\Delta - \gamma_\lambda + \gamma_D].$$

and anomalous dimensions are given as

$$\gamma_D = \frac{g''}{8\pi(1+u)} \left[1 + \alpha - \frac{2\alpha}{1+u} \right], \quad \gamma_v = -\frac{\alpha g''}{8\pi(1+u)^2}, \quad \gamma_\lambda = \frac{\alpha g''}{8\pi(1+u)} - \frac{\lambda}{2\pi}.$$

The quenched regime corresponds to the $u^* = 0$ and also in this case there are four possible IR stable fixed points:

$$\begin{aligned} \textbf{FP 5:} \quad & g''^* = 0, \quad \lambda^* = 0; \\ & \Omega_1 = -2\epsilon, \quad \Omega_2 = -\eta, \quad \Omega_3 = 2\Delta \\ & \beta = 1; \\ \textbf{FP 6:} \quad & g''^* = 0, \quad \lambda^* = -4\pi\Delta; \\ & \Omega_1 = -2\epsilon, \quad \Omega_2 = -\eta, \quad \Omega_3 = -2\Delta; \\ & \beta = 1 + \Delta; \\ \textbf{FP 7:} \quad & g''^* = 8\pi\epsilon, \quad \lambda^* = 0; \\ & \Omega_1 = 2\epsilon, \quad \Omega_2 = -\eta + \epsilon(1 - \alpha), \quad \Omega_3 = 2\Delta + \epsilon(1 - 2\alpha); \\ & \beta = \frac{2 - (1 - 2\alpha)\epsilon}{2 - (1 - \alpha)\epsilon}; \\ \textbf{FP 8:} \quad & g''^* = 8\pi\epsilon, \quad \lambda^* = 2\pi[-2\Delta + \epsilon(2\alpha - 1)]; \\ & \Omega_1 = 2\epsilon, \quad \Omega_2 = -\eta + (1 - \alpha)\epsilon, \quad \Omega_3 = -2\Delta + (2\alpha - 1)\epsilon; \\ & \beta = \frac{2 + 2\Delta}{2 - (1 - \alpha)\epsilon}. \end{aligned}$$

The nontrivial case occurs when no special choice for parameter u is considered, i.e. let's consider u finite and non-zero. Solving equations (10) for $u \neq 0, g \neq 0$ the following values for the coordinates of the fixed point are obtained

$$\frac{g^*}{8\pi u^*(1+u^*)} = \frac{2\epsilon - \eta}{1 + \alpha}, \quad u^* = -1 + \frac{\alpha(\eta - 2\epsilon)}{(1 + \alpha)(\eta - \epsilon)}. \quad (12)$$

The two possible regimes are distinguished by the value of the coordinate λ^* . Fixed point with zero value is given by

$$\textbf{FP 9:} \quad \lambda^* = 0, \quad \beta = \frac{2 - \eta + \alpha(1 + \epsilon - \eta)}{(1 + \alpha)(2 - \eta)}$$

and is stable in the region

$$(1 - \alpha)\epsilon < \eta < \epsilon, \quad \Delta + \frac{(1 + 2\alpha)\eta}{2(1 + \alpha)} > \frac{\alpha\epsilon}{1 + \alpha}. \quad (13)$$

The fixed point with non-zero value of λ^* is given by

$$\mathbf{FP\ 10:} \quad \lambda^* = -4\pi\Delta + \frac{2\pi\alpha\epsilon}{1 + \alpha} - 2\pi\eta\frac{1 + 2\alpha}{1 + \alpha}, \quad \beta = \frac{2 + 2\Delta}{2 - \eta},$$

and is stable in the region

$$(1 - \alpha)\epsilon < \eta < \epsilon, \quad \Delta + \frac{(1 + 2\alpha)\eta}{2(1 + \alpha)} < \frac{\alpha\epsilon}{1 + \alpha}. \quad (14)$$

5 Conclusions

Fixed points **1** and **5** corresponds to the non-interacting (mean-field or Gaussian) theory and thus their predictions should agree with the ones of rate equation approach, which is indeed the case [4].

From the fixed points' structure some physical consequences can be deduced. First we see, that compressibility has direct influence on the value of decay exponent (see **FP 3**, **FP 7-9**). For some regimes (**FP 3**, **FP 7**) it could lead to the enhancement (for both of them $\beta > 1$) of the reaction process compared to the corresponding regimes for incompressible case [6, 18]. As was already pointed this fact can be explained by the presence of compressible sinks into which particles are attracted (see also Sec. 4 in [24]). However we also observe that when both density fluctuations and compressibility are relevant (**FP 4**, **FP 10**), the density tends to suppress the influence of compressibility.

The “real problem” corresponds to the choice $\epsilon = \eta = 4/3$, which leads to the famous Kolmogorov “five-thirds law” [16] for the spatial velocity statistics. It is easy to see, that this regime can be realized either by the fixed point **FP 9** or **FP 10** depending on the value of parameter Δ , or equivalently on the space dimension d . From (13) and (14) we see that there is a “critical” value $\Delta_c = -2/(3 + 3\alpha)$ for the parameter Δ , above which **FP 9** is stable, whereas below it **FP 10** is stable. Because α is positive quantity, a parameter Δ_c is negative. Therefore in the vicinity of the space dimension two ($\Delta = 0$) regime represented by the fixed point **FP 9** should be realized with the decay exponent $\beta = (1 + 3\alpha)/(1 + \alpha)$. Thus we can conclude, that

compressibility has a profound effect on the large-scale asymptotic behavior of the annihilation process and leads to the enhancement of it near its critical dimension $d_c = 2$. On the other hand density fluctuations leads again to the suppression of compressibility (as can be seen by direct numerical inspection of exponent β for **FP 10**).

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